CMIST: A PORTABLE TOOL FOR IN SITU SAMPLE SCREENING AND SITE CHARACTERIZATION ON THE MOON

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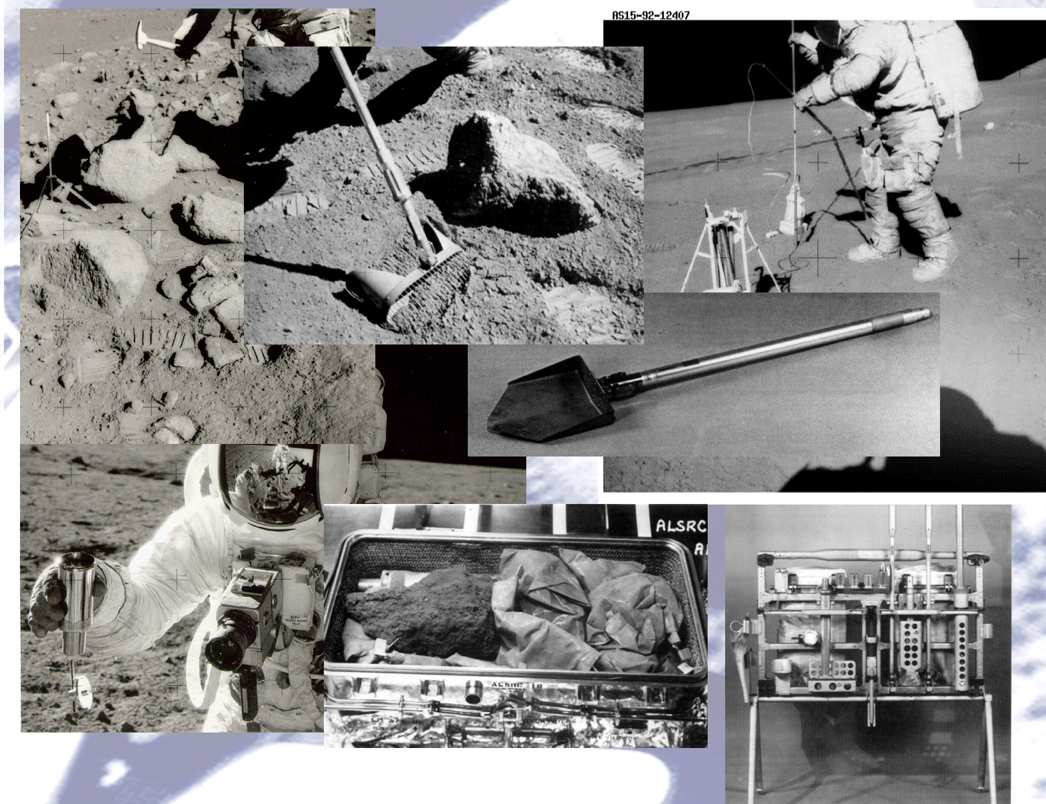
Tool and Instrument Time Needs on the Moon Then and Now

Manual sampling tools worked well, except for drills, and designing drills to within mass and power constraints is challenging, so need tools to sample stratigraphy by taking advantage of natural excavation process

Nothing but naked eye to describe samples which were then returned to Earth, but now limited returnable mass and longer stays, so need tools for 'down select' for Earth return or in situ analysis.

Documentation relatively cumbersome for much shorter stays, so need to enhance data capture, information access on demand.

Combined, portable XRF/XRD requiring minimal to no sample preparation, could meet that need.



Breakthrough Field Tool based on combined XRF and XRD

CMIST: Chromatic Mineral Identification and Sample Texture

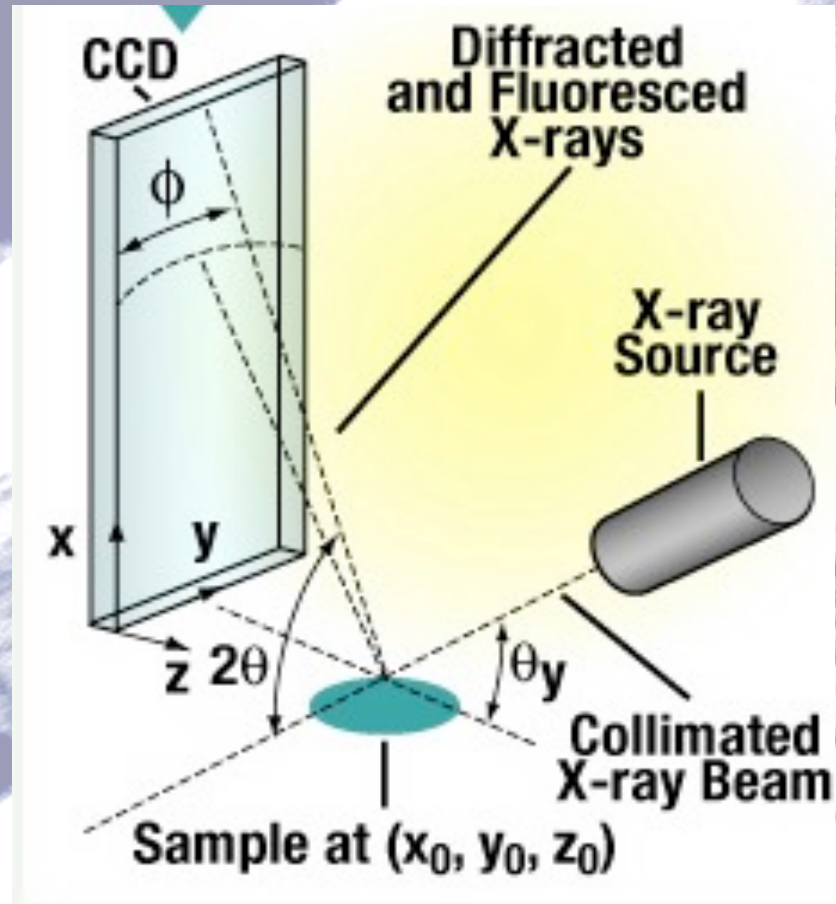
To map a rock's element and mineral abundance and relationships grain by grain to understand its origin in real time

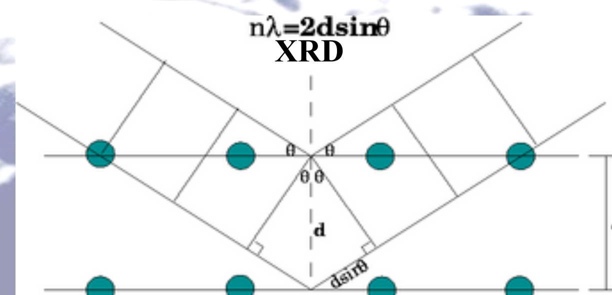
Comprehensive analysis with no sample preparation based on breakthroughs in X-ray instrument components for High Energy Astrophysics.

Source: Continuum rather than monochromatic so larger range of input wavelengths creates much greater range of detectable d-spacings for same 2θ, increasing probability of diffraction for untouched grains.

Detector: Low Noise, deep depletion, single photon counting CCD, recording time of event as well as energy and position in 3D, with optical wavelength sensitivity, allowing simultaneous optical (CCD) imaging to identify source on sample.

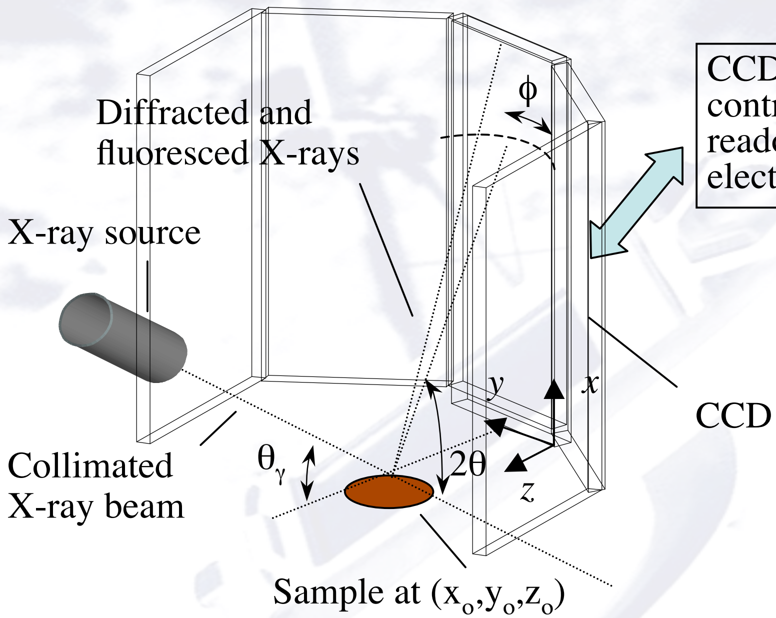
Analysis: rapid simultaneous xrf/xrd analysis by modifying XSPEC software tool for 2D fitting (E vs either d or 2θ)





Multi-Dimensional XRF/XRD capabilities for greatly enhanced analysis

CCDs provide energy (wavelength) and position information for individual photons. Using continuum radiation literally opens up a new dimension. The richness of the resulting data is surprising…



CCD control and readout electronics ⟷ Computer interface with event processing

Four-dimensional event list:

time, x, y, energy

for each detected X-ray

Apply geometry

time, θ, φ, λ

for each event

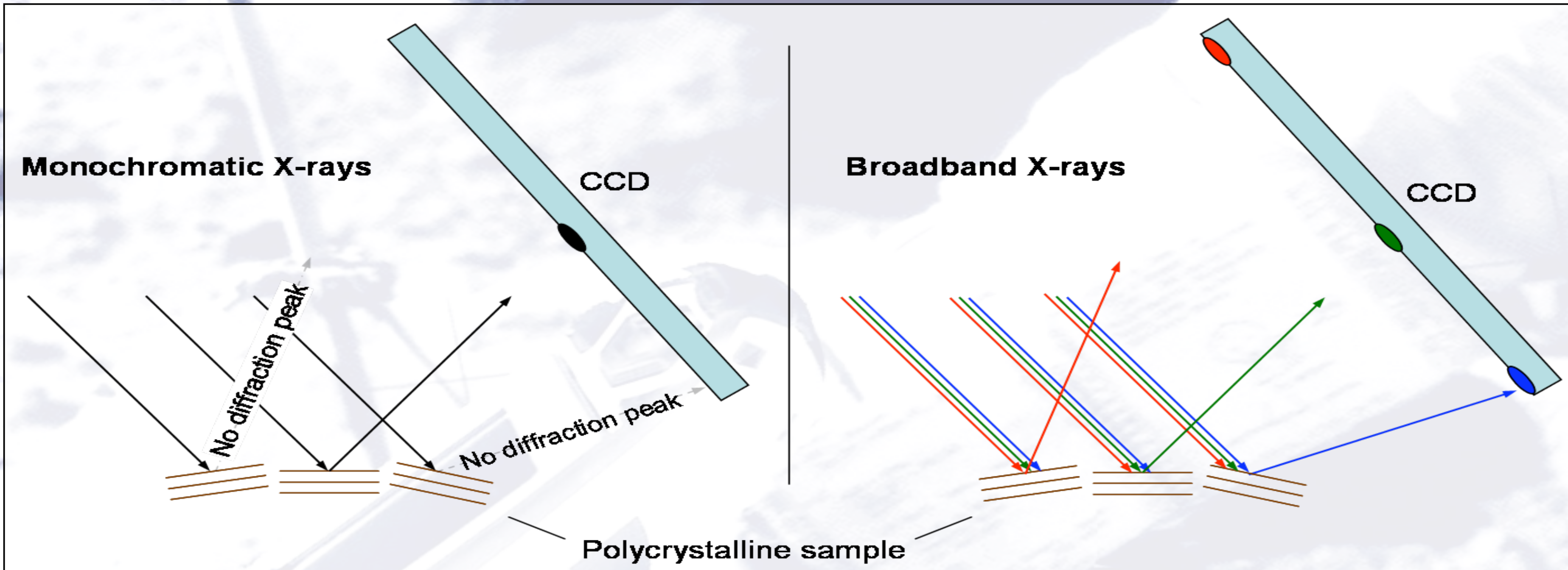
Apply Bragg's law,
$n\lambda = 2d \sin(\theta)$

time, d-spacing, orientation, energy

for each event.

An X-ray source producing Bremsstrahlung continuum X-rays (0.1-10 keV) sends a collimated beam toward a sample. The X-rays either diffract from atomic planes in the sample or excite characteristic line emission. A photon-counting, energy-resolving CCD captures some of the resulting X-rays, producing an event list that can be transformed into both fluorescence (elemental composition) and diffraction (mineral atomic-plane spacing) information on an event-by-event basis.

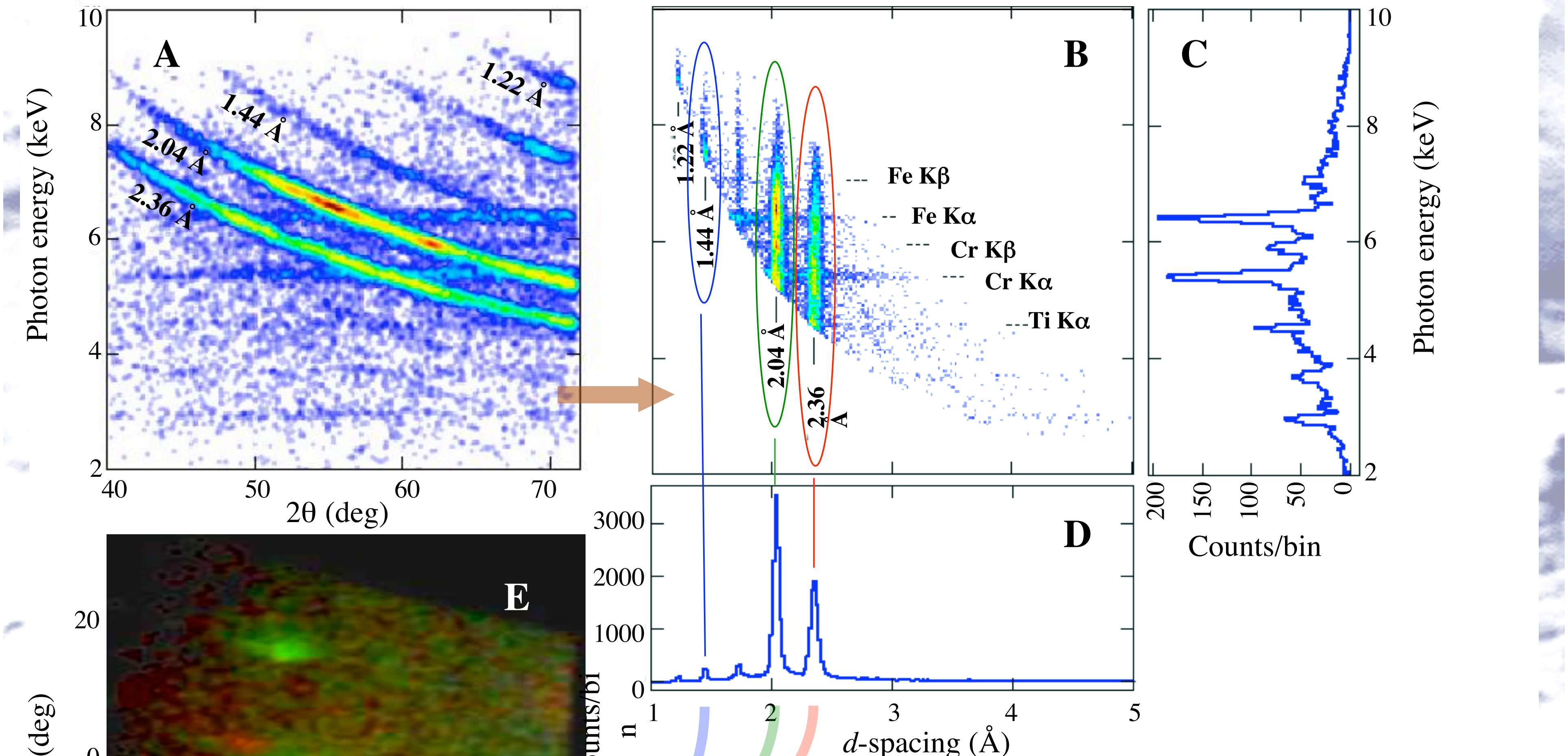
Different from Monochromatic X-ray



The use of a Broadband wavelength source allows capture of the range of crystal orientations present on the 'raw' sample with a finite length CCD, enhancing *CMIST* ability to probe crystal structure (right). Monochromatic X-rays (left) strike sample containing crystallites of given atomic plane spacing, d, with range of orientations. Bragg's law fixes relationship between d, diffracted angle, and wavelength with resulting constructive interference from only one crystallite.

Continuum X-rays for XRD gives more d-space range for fixed geometry

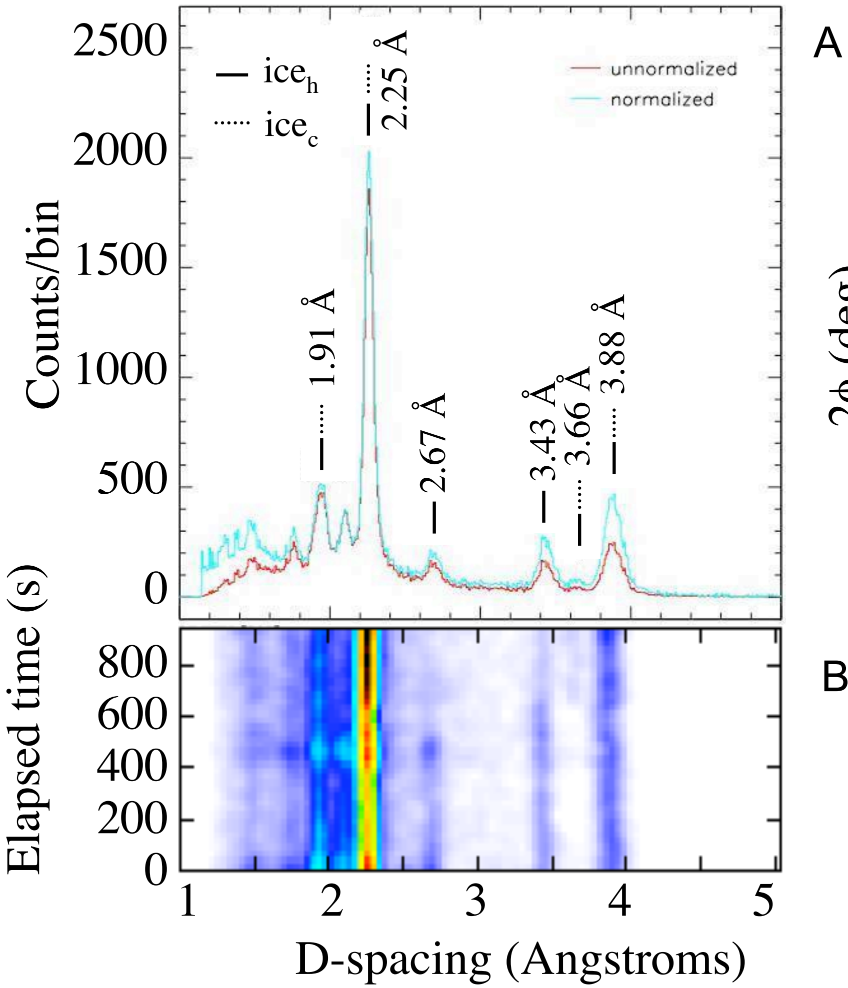
Demonstration of CMIST Capability for Bulk Sample Analysis

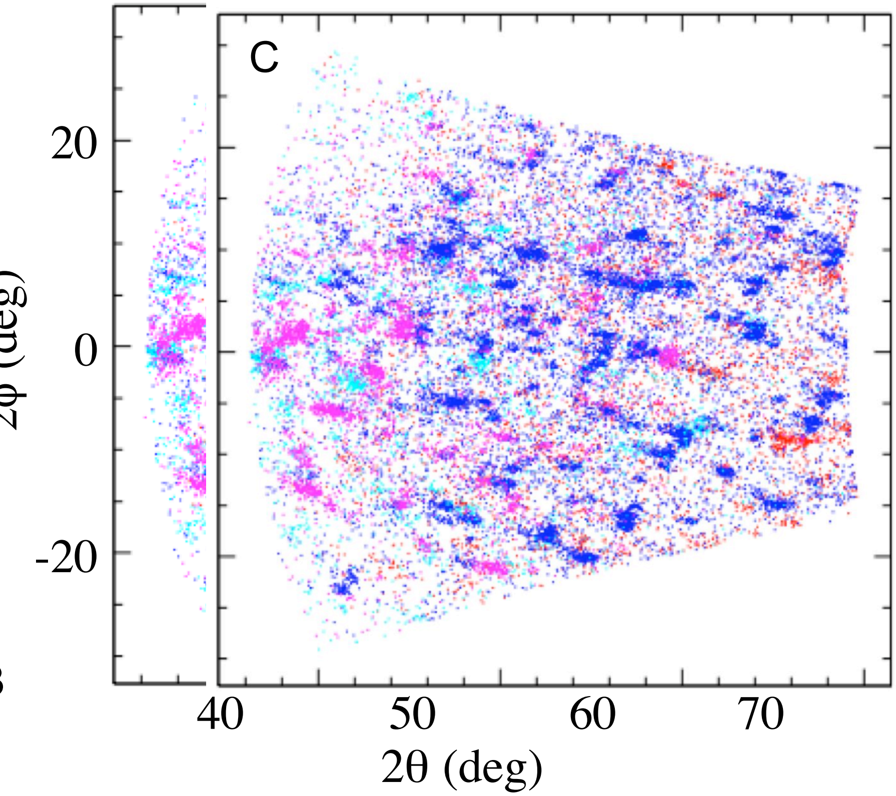


CXRDF data for a bulk Al 6061 sample. *Panel A:* Photon count intensity binned in energy and diffraction angle 2θ. Horizontal features represent X-ray fluorescence from elements (here, contaminants) found in the sample; arcs correspond to diffraction from discrete atomic plane spacings (Miller indices), tracing out Bragg's law for $n = 1$. *Panel B:* Photon counts binned in energy and *d* value. Fluorescence features and *d*-spacings for aluminum are indicated. *Panels C, D:* Energy (*vert.*) and *d*-spacing (*horiz.*) spectra. *Panel E:* Spatial image of specular-diffracted X-ray intensity, in angular coordinates depicting the orientations of crystallite lattice planes (hkl) = (111), (200), and (220).

Demonstration of CMIST for Volatile Materials

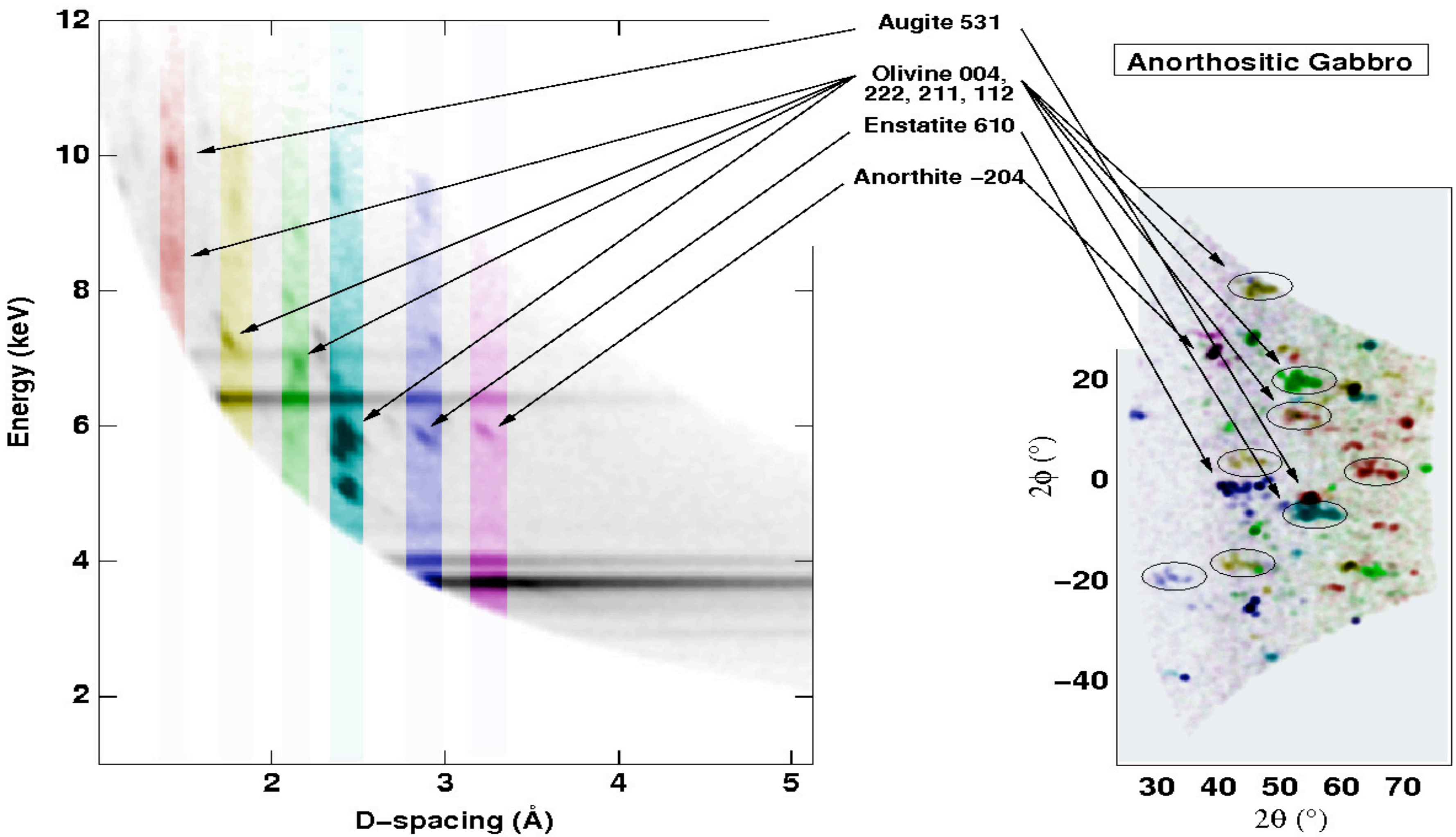
Water Ice: XRD from frost collected on LN2 cooled container. Possible transitions between cubic and hexagon ice seen in data vs time.



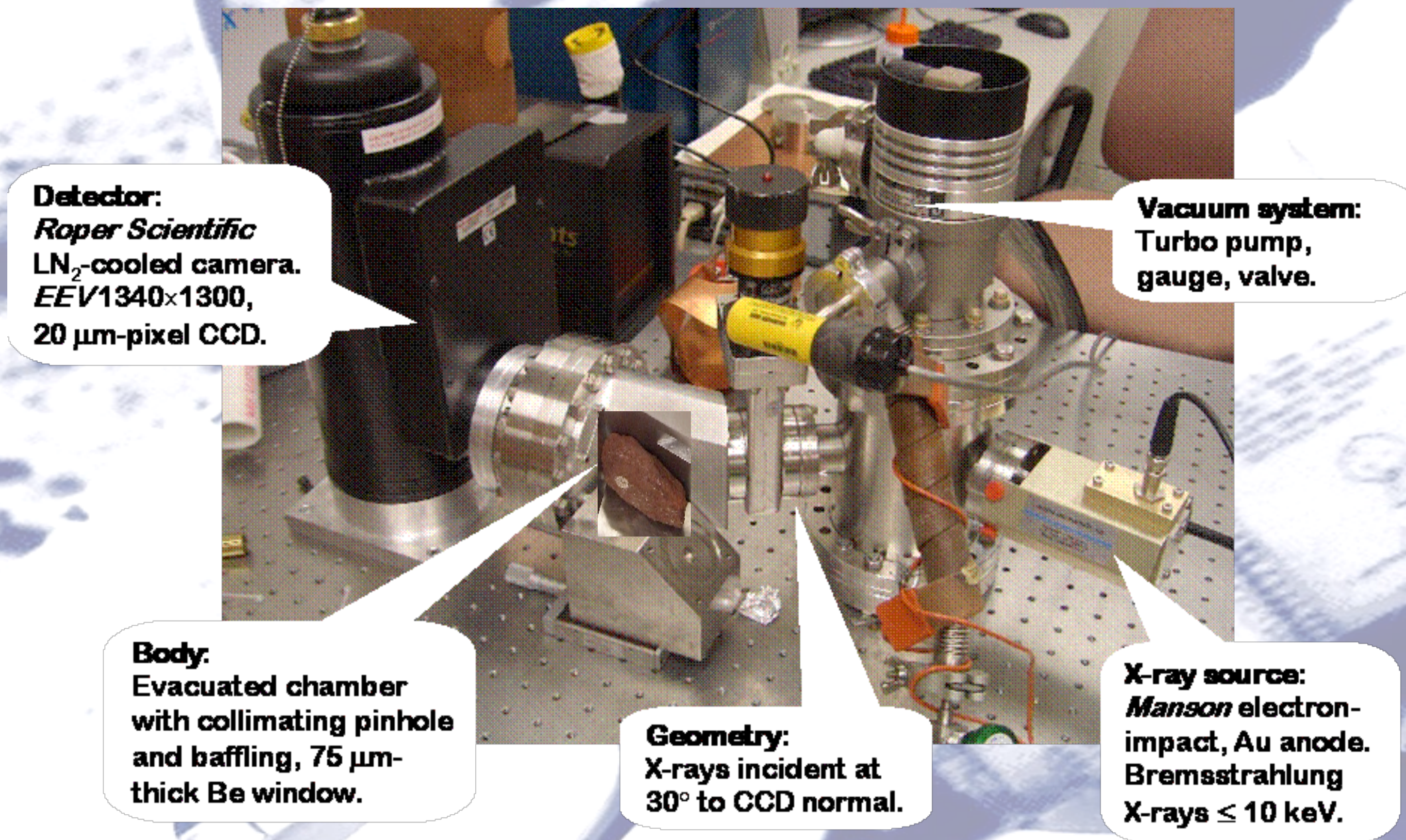


CXRDF data for frost. *A:* *d*-spacings for hexagonal and cubic ice. *B:* Time dependence of d-spacings. *C:* Scatter-plot of photons in angular coordinates, for d values 1.91, 2.25, 3.43, 3.88 Å. Spots are grains a few hundred μm in size.

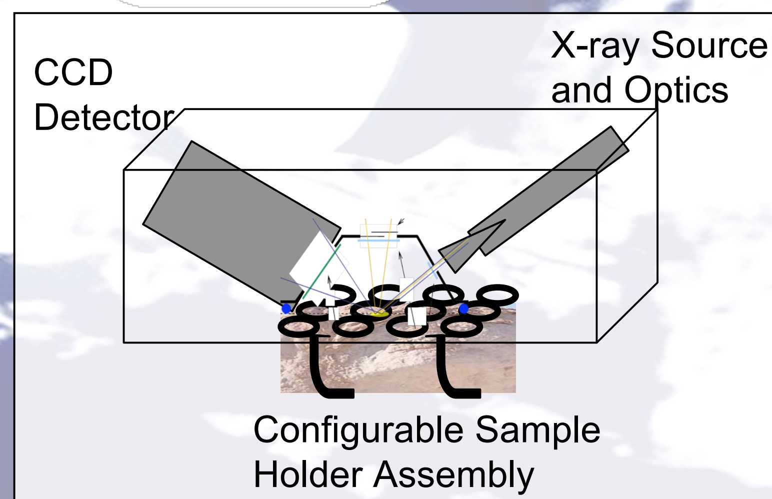
First Demonstration of CMIST on Lunar Analogue Rock



Identifying minerals from completely unprepared known sample of anorthositic gabbro of small to moderate grain size showing CMIST capability to distinguish and characterize phases for anticipated minerals. Color coded d-spacings (left) distinguish major minerals by miller index. Map of crystal orientations (right) shows Laue spots of the mineral grains, including the morphology of an olivine crystal (circled).



From Laboratory to Portable Version

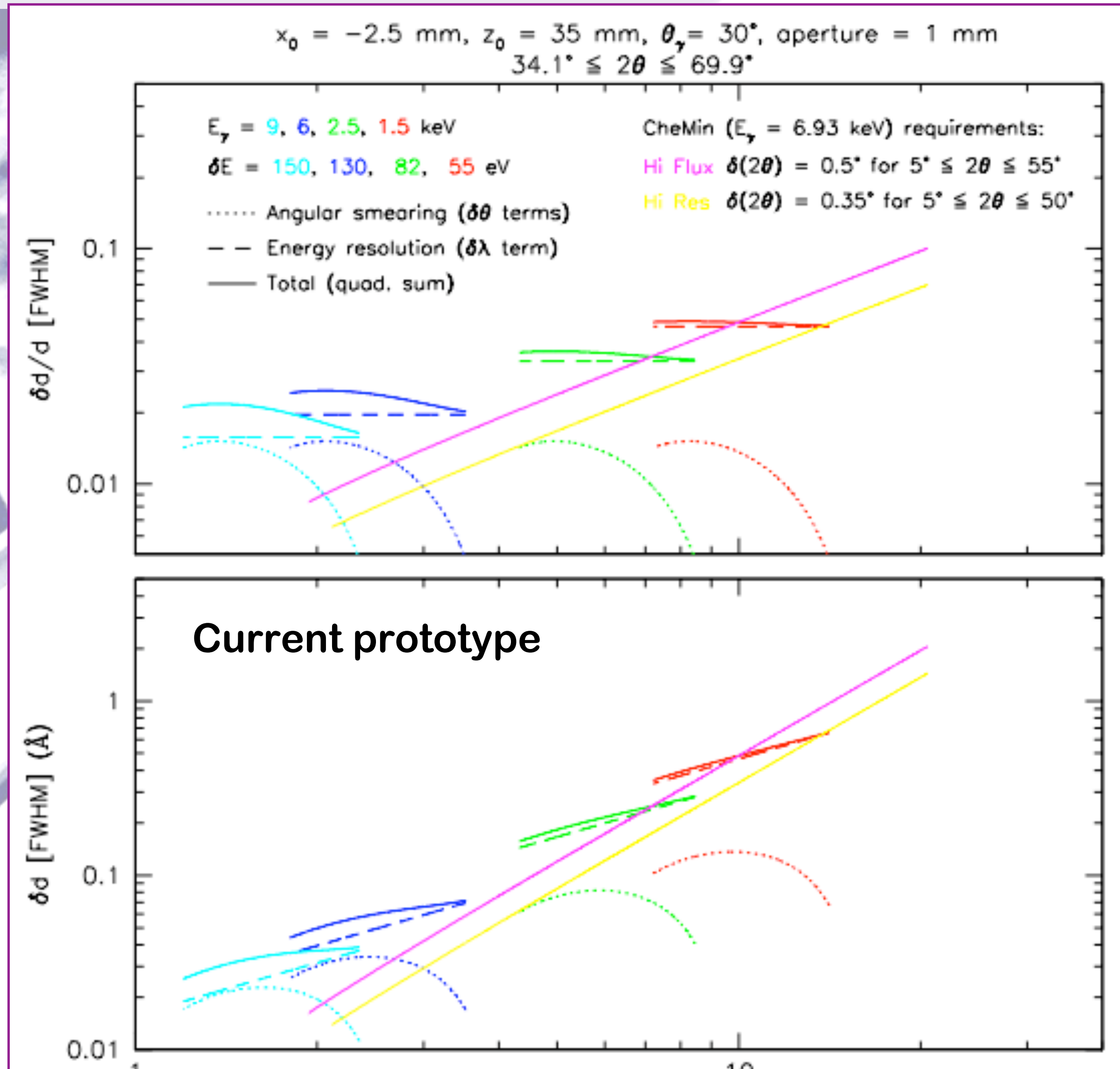


Projected Improvement in D-Spacing Range and Resolution Capabilities

D-spacing resolution is a function of energy resolution and geometric terms.

Current prototype attempts to equalize these terms with CCD at 35 mm from sample and 1 mm diameter illumination size. Larger effective X-ray 'pinhole' increases throughput at expense of some loss of resolution.

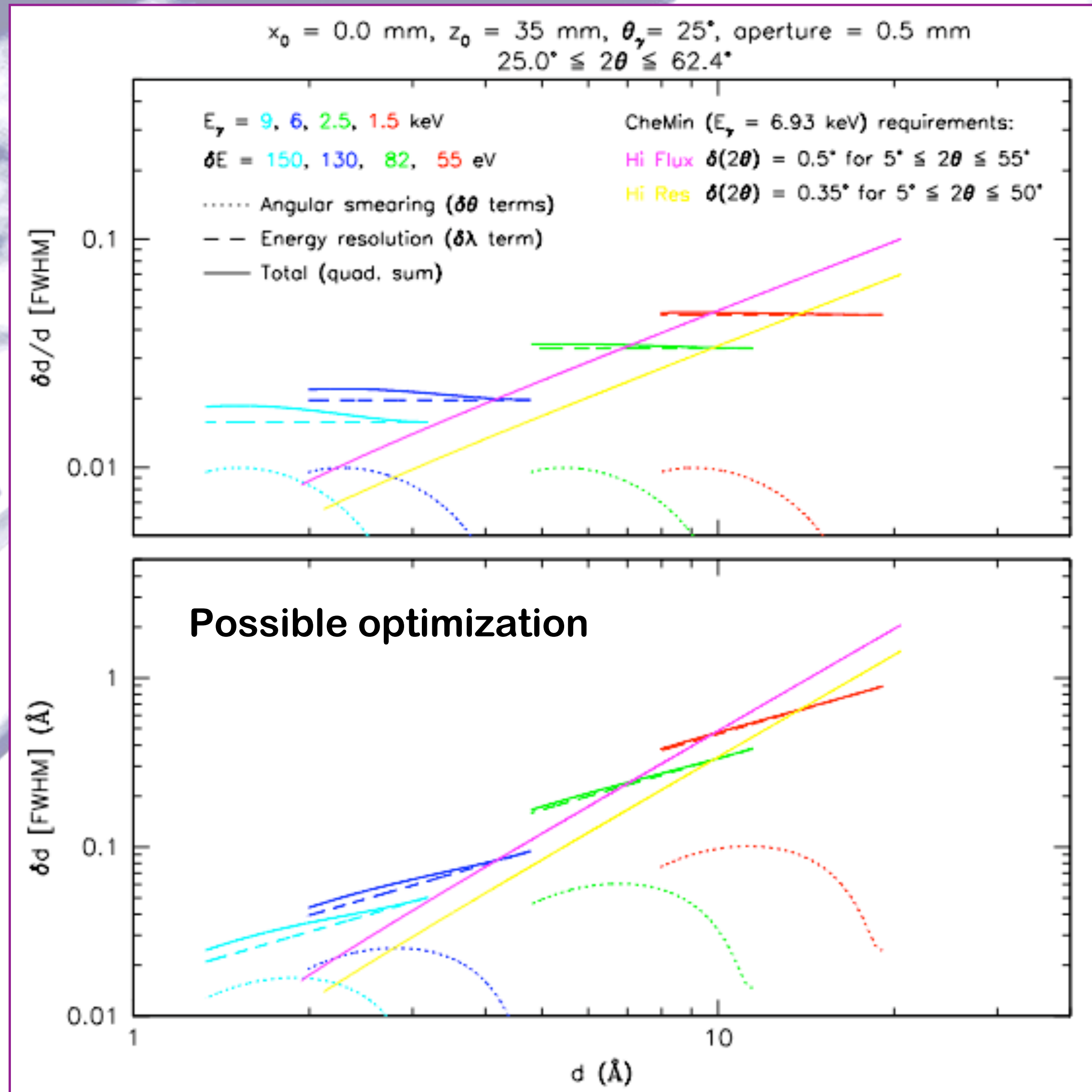
While d-spacing resolution is less than for Chemin, it does have a much larger throughput for same source power.



$$\left(\frac{\delta d}{d}\right)^2 = \left(\frac{\delta\lambda}{\lambda}\right)^2 + \left(\frac{\delta\theta}{\tan\theta}\right)^2$$

Possible optimization of design where geometric terms in d-spacing resolution are minimized.

In this case, sample is about 35 mm away from CCD and the illumination size is about 0.5 mm diameter.



Science Capability Compared to CHEMIN

- Unaltered particle/domain size and orientation distributions
  Information about sample volcano-tectonic or impact origin and history (petrology): pressures, temperatures, stresses, magnetic fields, shock metamorphism
- In Situ Water ice measurement capability
  Since we would not need to grind and possibly melt/evaporate the ice
- Portability, minimal power and mass, not limited by sample tray or moving parts
- Higher throughput for same power, large d-spacing range, at expense of somewhat less d-space resolution
- Multi-functionality capability for rock, volatile, or surface analysis tool
- Use as real time handheld sample and/or rover-mounted traverse instrument

Future work

- Use X-ray astrophysics optimized CCDs
  - •MIT LL device (Suzaku model)
  - •Osaka University/ Hamamatsu p-channel device
  - •Implement new radiation hardening techniques

•Use new Low power/ low noise/ high speed output chain ASIC

•Integrate new GSFC modulated X-ray source

•Implement astrophysics-like forward fitting by adapting XSPEC to multidimensional analysis to look for weak signals buried in noise.

•Perform analysis on sample suites exhibiting systematic changes in textures and grain sizes across flow fronts or ejecta blankets collected from traverses at one or more identified (NASA MMAMA program) terrestrial analogue for the Moon and Mars

Backup Slides

The Future of XRD Instrumentation

Table 1: Systematic Improvements in XRD Instrument Capabilities			
Measurement	***CheMin***	***MICA***	***CMIST***
Mineral ID diffraction geometry d-spacing range d-spacing res. @2.5, 5, 10A	Monochrom. powder diff. transmission 2-35A 0.035A, 0.1A,0.5A	Monochrom. diffraction reflection 1.8-6A unknown, unknown, N/A	Multi-λ diffraction reflection 1.3-24A 0.065A, 0.2A, 0.5A
XRF Elemental ID range speed/ efficiency	1-6.5 keV low	1-5.5 keV low	0.25-12 keV high
X-ray Source	Mono-energetic	Mono-energetic	continuum
Sample Handling moving parts homogenized sample characterize crystallite ID of water ice shock metamorphism	grind, sift, align, discard with grinder, sifter, arm always never never can probe	no preparation, arm, abrasion tool desirable optional in limited way Yes can probe Can probe	no preparation, arm, abrasion tool desirable optional yes Yes can probe Can probe
X-ray Detector flight heritage format, pixel size room temperature	CCD (E2V) XMM-Newton, Swift 600x600, 40 μ No	CCD (unknown) unknown unknown No	CCD (MIT or Suzaku) ASCA, Chandra, HETE2 2048x2048, 3 cm Yes when fully implemented
Other Capabilities	None	sample optical imaging	sample optical imaging